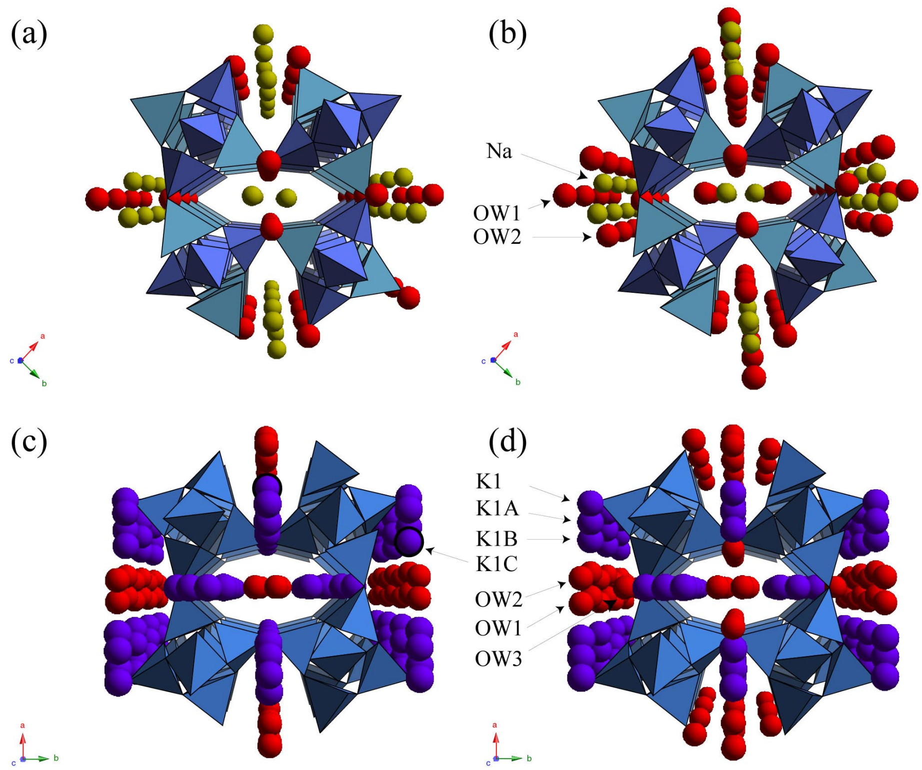
Abstract No. lee0343

Pressure-Induced Hydration and Cation Migration in a Zeolite

Y. Lee, T. Vogt (BNL, Physics), J.A. Hriljac (Univ. Birmingham, UK), J.B. Parise (SUNY, Stony Brook), J.C. Hanson (BNL, Chemistry), S.J. Kim (KIST, Korea)

Beamline(s): X7B, X7A

The aluminosilicate zeolite natrolite has recently been shown to undergo a reversible volume expansion and superhydration in the presence of water and under hydrostatic pressure above 1.2 GPa.[1] At high pressure this superhydrated natrolite contains twice as many water molecules as under ambient conditions, which form hydrogen-bonded water “*nano-tubes*” inside the zeolitic channels that contain the charge-balancing sodium cations. This constitutes to our knowledge the first experimentally observed water nanotube after the recent MD simulation results of water in carbon nanotubes and the first example of pressure-induced formation of nanotube arrays within zeolite hosts. Upon pressure release the extra water molecules are released. A “high-pressure sponge” capable of remaining in its superhydrated state *after* pressure is released might have useful technological applications, as well as being a model system to study the water structure at the nanoscale. Here we show that a gallosilicate analogue of natrolite is such a system and does indeed remain in a superhydrated state upon pressure release from 1.9 GPa.[2] A single crystal study of the recovered gallosilicate natrolite shows that the material contains twice as much water as before superhydration.[3] These water molecules arrange differently than in the related aluminosilicate material, forming hydrogen-bonded water “*nano-chains*” inside the zeolitic channels. The results suggest that the water nano-structures can be further tailored as a function of the framework and non-framework chemistry of zeolitic nanopores and irreversible superhydration, albeit at lower pressures, has the potential to trap pollutants such as radionuclides or small molecules (e.g. tritiated water).



Acknowledgments: This work was supported by LDRD of BNL (Pressure in Nanopores). Research carried out in part at the NSLS at BNL is supported by the U.S. DoE, Division of Materials Sciences and Division of Chemical Sciences (DE-Ac02-98CH10886 for the X7A/B beamlines). We acknowledge the Geophysical Lab of the Carnegie Institute for allowing us the use of the ruby laser system associated with the beamline X17C.

References:

[1] Lee, Y.; Hriljac, J. A.; Vogt, T.; Parise, J. B.; Artioli, G. Journal of the American Chemical Society 2001, **123**, *12732-12733*.

[2] Lee, Y.; Vogt, T.; Hriljac, J. A.; Parise, J. B.; Artioli, G. Journal of the American Chemical Society 2002, **124**, *5466-5475*.

[3] Lee, Y.; Vogt, T.; Hriljac, J. A.; Parise, J. B.; Hanson, J. C.; Kim, S. J. Nature *accepted*.

Figure. Polyhedral representations of Na-AlSi-NAT and K-GaSi-NAT before and after pressure-induced hydration. (a) Na-AlSi-NAT at 0.40 GPa, (b) Na-AlSi-NAT at 1.51 GPa, (c) as-synthesized K-GaSi-NAT and (d) K-GaSi-NAT recovered from 1.9 GPa. Tetrahedra in Na-AlSi-NAT are shown in two colours to illustrate the ordering of Al/Si over the framework tetrahedral sites whereas Ga/Si in K-GaSi-NAT are disordered and shown in one colour. K1C atoms are emphasized with bold outlines.